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The Numerical Nuclear Reactor for High Fidelity Integrated Simulation of Neutronic, Thermal-Hydraulic and Thermo Mechanical Phenomena – Project Overview

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As part of a US-ROK collaborative I-NERI project, a comprehensive high fidelity reactor core modeling capability is being developed for detailed analysis of current and advanced reactor designs. The work involves the coupling of advanced numerical models such as computational fluid dynamics (CFD) for thermal hydraulic calculations, whole core discrete integral transport for neutronics calculations, and thermo-mechanical techniques for structural calculations. The product code has been designed to run on parallel high performance computers. This integrated simulation capability will provide a verifiable computational tool to perform intensive studies on the operational and safety characteristics of various design alternatives and to compare the results obtained with presently available tools to those from this high fidelity capability. This paper provides an overview of the project and a summary of the key elements of the integrated code.

KEYWORDS: thermal-hydraulics, neutronics, coupled codes, computational fluid dynamics, CFD, integral transport theory, reactor physics, core analysis, high performance computing, parallel computers, numerical reactor

1. Introduction

A comprehensive high fidelity reactor core modeling capability is being developed for detailed analysis of current and advanced reactor designs as part of a US-ROK collaborative I-NERI project [1]. High fidelity is accomplished by integrating highly refined solution modules for the coupled neutronic, thermal-hydraulic, and thermo-mechanical phenomena. Each solution module employs methods and models that are formulated faithfully to the first-principles governing the physics, real geometry, and constituents. Specifically, the critical analysis elements that are incorporated in the coupled code capability are (1) whole-core neutron transport solution, (2) ultra- fine-mesh computational fluid dynamics/heat transfer solution, and (3) finite- element-based thermo-mechanics solution, all obtained with explicit (fuel pin cell level) heterogeneous representations of the components of the core. The vast computational problem resulting from such highly refined modeling will be solved on massively parallel computers, and serve as “numerical nuclear reactor”. Relaxation of

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modeling parameters are also being pursued to make problems run on clusters of workstations and PCs for practical applications as well.

Companion papers describe the details of the individual components in the areas of reactor physics, thermal-hydraulics and thermo-mechanics, coupling techniques for the solution of such multi-physics problems, and the results of initial coupled calculations. In each of the phenomenological areas, the objective is to develop and demonstrate the ability to calculate accurately the individual key phenomena. The integration of these high fidelity models into a robust computational tool, along with verification and validation of the integrated capability, would then provide the desired tool for advanced reactor design. The elements of the Numerical Nuclear Reactor and the lead organizations are indicated in Fig. 1. In each of the three key phenomenological areas, examination of numerical performance and verification/validation are being performed. For the coupled code, strategies and numerical performance have been investigated and validation of the code against integrated benchmarks will be initiated.

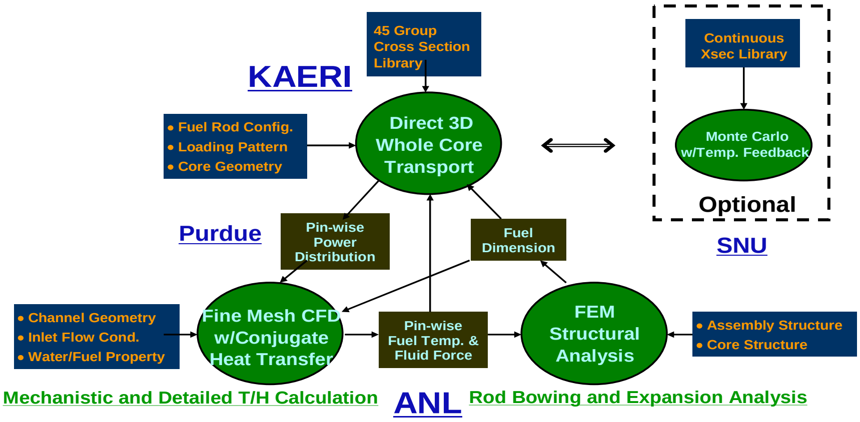


Fig.1 Numerical Nuclear Reactor Elements and Participants

2. Reactor Physics

The reactor physics module, being developed at KAERI, is a whole core transport code, DeCART (Deterministic Core Analysis based on Ray Tracing), based on the method of characteristics. [2,3] This code generates sub-pin level power distributions by representing local heterogeneity explicitly without homogenization, using a multigroup cross section library directly without group condensation and incorporating pin-wise thermal hydraulic feedback. Transient and depletion analysis capabilities will be implemented in the near future. In DeCART, the coarse mesh finite difference (CMFD) formulation is employed as the means of coupling 2-D and 1-D MOC (Method of Characteristics) solutions as well as accelerating the MOC solutions. Since it is impractical to apply directly three-dimensional ray tracing to whole core problems, decoupling the 3-D problems into planar (2-D) and axial (1-D) problems was considered from the beginning of the code development.

First year activities were directed toward development of the 3D heterogeneous core transport calculations capability, and incorporation of thermal-hydraulic feedback in the steady-state solution scheme. As part of the efforts to verify this module, a Monte Carlo computational scheme with pin-by-pin thermal hydraulic feedback capability, known as MC-CARD [4], has also been developed by partners at Seoul National University. Recent activities have focused on parallel execution capability, verification of solutions and assessment of conventional neutronics solutions. The major calculation modules (ray tracing, CMFD and multi-group microscopic cross section manipulations) have been parallelized and full distributed memory allocation employing axial domain decomposition has been accomplished. Parallel efficiency of approximately 80% with 24 processors on a LINUX cluster has been achieved.

Comparisons between conventional methodologies on benchmark problems, fuel assemblies, and whole core calculations indicate excellent performance in terms of accuracy and computational time. Figure 2 illustrates the excellent agreement between DeCART and MC-CARD for the 3D mini-core problem.

Case	k-eff			Pin Power Error		Fr	
	MCCARD	DeCART	Error, pcm	RMS	Max. Rel (%)	MCCARD	Error (%)
HZP	1.22526	1.22091	-291	0.42	1.79	2.364	-0.02
HFP	1.19692	1.19358	-234	1.52	3.96	2.041	0.98

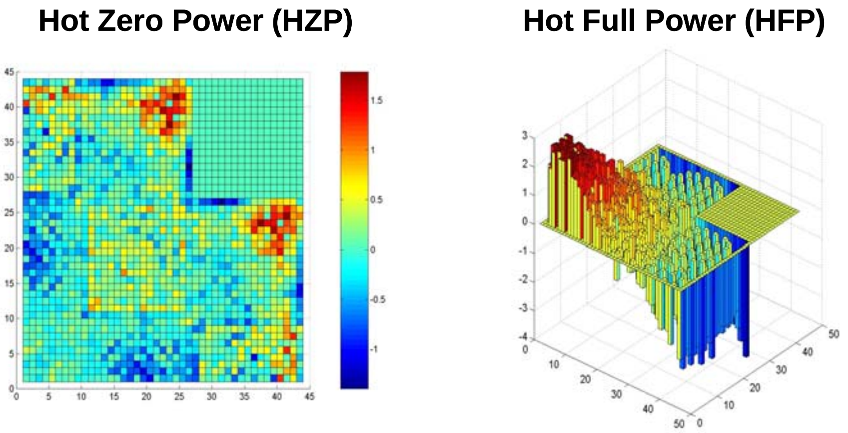


Fig.2 Comparisons between DeCART and the MC-CARD Monte Carlo Calculations for a 3D "Mini-Core". DeCART Pin Power Error (0%) for the HZP and HFP Minicore Cases.

3. Thermal-Hydraulics

Thermal hydraulic analysis has been focused on the use of high fidelity computational fluids dynamics capabilities available in several commercial CFD software, with specific focus being applied to the STAR-CD[5] and CFX[6] codes. While it is recognized that these CFD codes have the theoretical capability of simulating events at fine detail in a reactor application, a demonstration of their ability to predict observed flows in rod bundle geometry was considered critical for their ultimate inclusion in the integrated code system. It is believed that such codes have a sufficient range of turbulence and heat transfer models that they can be applied successfully to both current reactors and advanced reactors, such as those being considered in the Generation-IV program. Nonetheless, proof of this capability became a key project objective, with initial focus on water and gas cooled systems. Project efforts at ANL and KAERI have thus focused on experimental validation of these codes, with particular emphasis on demonstrating their ability to predict turbulent flow and associated heat transfer in rod bundle flows.

Initial thermal-hydraulics activities focused on a review of commercial CFD capabilities for high fidelity thermal-hydraulic analysis of light water reactors. Independently, an evaluation of CFD turbulence models has been performed at ANL and KAERI for modeling turbulent flow and heat transfer in fuel rod bundle geometries[1,7,8]. A numerical simulation of the turbulent flow structure was performed for a square base rod bundle. The evaluation of various Reynolds-Averaged Navier-Stokes (RANS) models--including the standard k-ϵ model, quadratic and cubic k-ε models, and the renormalization-group (RNG variant) for rod bundle flow indicated strengths and weaknesses of each method. The second-order moment closure models such as the differential Reynolds stress model (RSM) were also evaluated.

More recently, analyses have focused on an experimental study by Krauss and Mayer [9] of turbulent transport of momentum and energy in heated rod bundles. The numerical analysis has been performed to simulate not only turbulent flow but also heat transfer for the rod bundles using various RANS turbulence models: standard κ-ε model, non-linear quadratic κ-ε model (Speziale), and Reynolds stress models (Launder-Reece-Rodi, Speziale-Sarkar-Gatski). Example of results are shown in Figure 3, which compares the predicted normalized wall shear stresses along rod surface by turbulent models for the P/D=1.06 and 1.12 cases. Except for standard k-ε, remaining turbulent models show similar predictions with reasonable accuracies. However, the prediction results became worse as P/D ratio decreases.

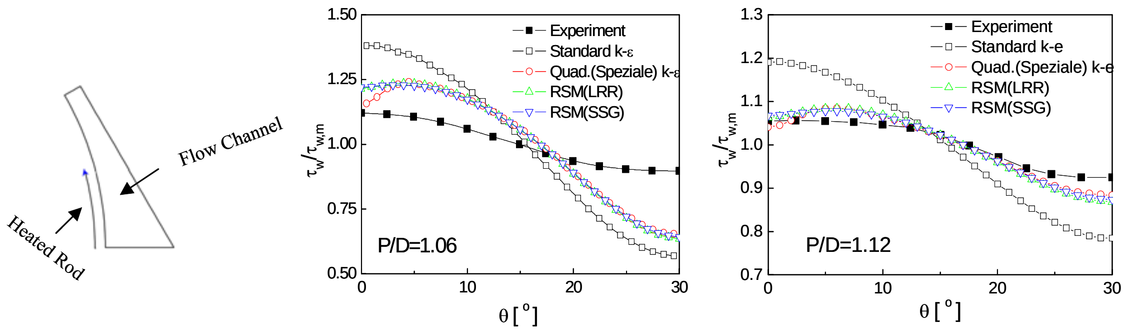


Fig.3 Normalized Wall Shear Stress Distributions

Although completely accurate prediction of turbulent structures in the subchannel have not been demonstrated, prediction of heat transfer coefficients, considered critical for these applications, was good for forced flow applications. RANS models were used to compute the heat transfer coefficient for flow in a tube and compared with the values predicted by the well-known Dittus-Boelter correlation; h_{DB} = (k/d) 0.023 $Re^{0.8}$ $Pr^{0.4}$. The tube used in this analysis has a diameter equal to the hydraulic diameter of a typical PWR flow channel, and the flow parameters were set to values that are typical for PWR reactors at operating conditions from 100% to 5% of full-power.

In Table 1, the heat transfer coefficient computed at the wall by the k-ε model on the basis of the bulk coolant temperature (h_{CFD}) is compared with the heat transfer coefficient computed by the Dittus-Boelter correlation (h_{DB}). In summary, the discrepancy between the heat transfer coefficient computed by the k-ε model and the value predicted by the Dittus-Boelter correlation is about 4% to 11% for the range of Re numbers from ~25,500 to 510,000. Analyses were also performed with the RNG model and a two-layer k-ε model for the case of Re = 254,809. The results suggest that the fine resolution of the boundary layer provided by the two-layer model results in a better agreement with predictions of the Dittus-Boelter correlation; however, the high Re number k-ε model predictions are within the experimental error.

4. Thermo-Mechanics

The third phenomenological element of the integrated code relates to modeling of thermo-mechanical response. For conventional reactor applications, coupling of the thermo-mechanical and thermal hydraulics analyses can be used to assess, for example, the effects of rod bowing on flow and heat transfer, which may affect assessments of departure from nucleate boiling. In advanced reactors, where inherent safety characteristics may depend on structural and neutronic response to thermal transients, the ability to closely couple the three phenomena may lead to clearer demonstration of inherent safety or a reduction in overly conservative safety margins.

Table 1 Heat Transfer Coefficient Comparisons

	Distance from inlet	h_{CFD} W/(m^{2}C)	h_{CFD}/h_{DB}
Re = 509,619	0.20 m	39,300	0.930
	0.30 m	39,448	0.933
	0.40 m	39,890	0.943
	0.45 m	39,984	0.946
Re = 254,809	0.20 m	22,096	0.910
	0.30 m	22,257	0.917
	0.40 m	22,522	0.927
	0.45 m	22,553	0.929
Re = 127,405	0.20 m	12,353	0.886
	0.30 m	12,605	0.904
	0.40 m	12,948	0.928
	0.45 m	12,943	0.928
Re = 25,481	0.20 m	3,680	0.956
	0.30 m	3,643	0.947
	0.40 m	3,626	0.942
	0.45 m	3,620	0.941

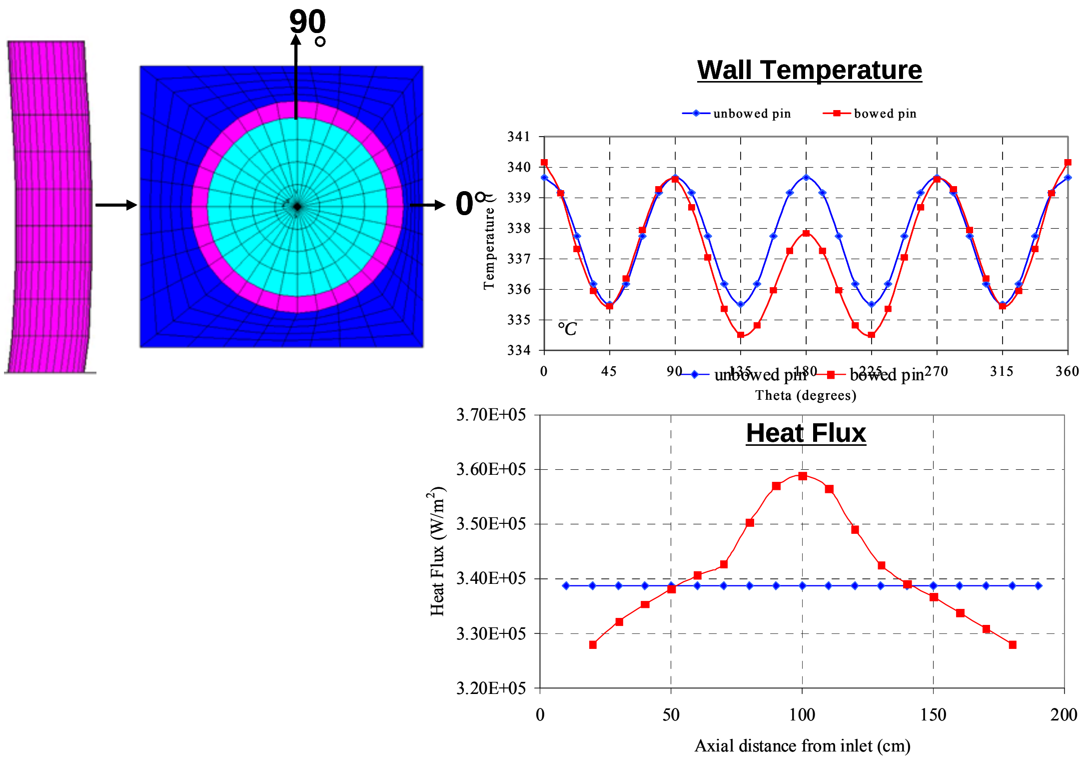


Fig.4 Effects of Fuel Rod Bowing Comparison of Temperature and Heat Flux Profiles at Cladding-Coolant Interface in the Directions of Bowing for the Straight and Bowed Pin Cases (with axially uniform heat generation)

The project is using a three dimensional finite element code, NEPTUNE [10], developed at Argonne to simulate the response of reactor components to design basis and beyond the design basis loads. The element formulations can properly treat large deformations and the rate-type material models can handle large material strains. Figure 4 illustrates the importance of rod bowing effects in a PWR pin at steady state conditions. Prediction of such geometric effects on flow passages are expected to be important in both steady-state and transient analysis, providing guidance on changes in the DNB limits and help quantification of DNB penalties.

5. Coupling Methodology

The ultimate objective of this effort is to produce an integrated analysis capability for these multi-physics models, having demonstrated the validity of the individual components. General purpose coupling schemes have been developed within the project as illustrated in Figure 5 and compared among them for quality assurance. [11] Iteration strategies for exchange of relevant information among the modules are being investigated, demonstrating, for example the importance of proper mapping between the neutronics and thermal hydraulics grids, which are vastly different. The coupling of CFD and MOC is generally very different than conventional LWR coupled code projects of the past since the reduced mesh sizes in CFD and MOC leads to considerably larger data transfer and more complex mapping requirements. The thermal-hydraulics meshing of conventional LWR system codes such as RELAP-5 and TRAC-M is much coarser than CFD meshing.[12] In the core models used in the conventional thermal-hydraulic systems codes, several neutronics mesh are generally assigned to a single thermal-hydraulic node. For example, in the core model used for the PWR core in the RELAP5 model of TMI used in the OECD Main Steam Line Break benchmark problem, 152 thermal-hydraulic nodes were used to model the entire core which consisted of 193 fuel assemblies.[13] Conversely, millions of computational cells are being used in STAR-CD to model a single fuel assembly. In the nodal neutronics model of the TMI core, 5400 zones were used to model the 193 assemblies, whereas 166,000 zones are being used in the DeCART model of a single fuel assembly.

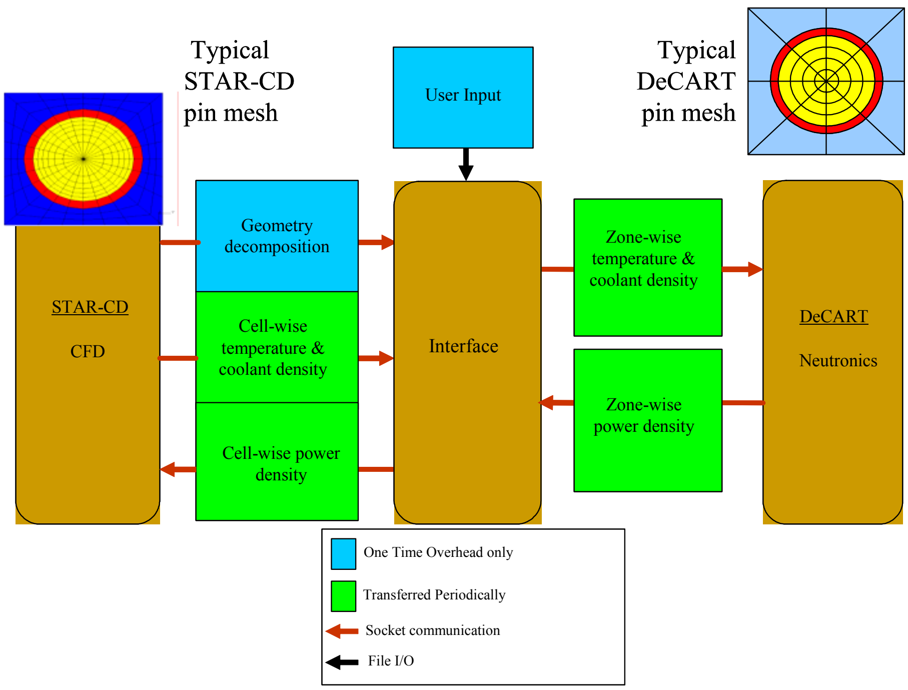
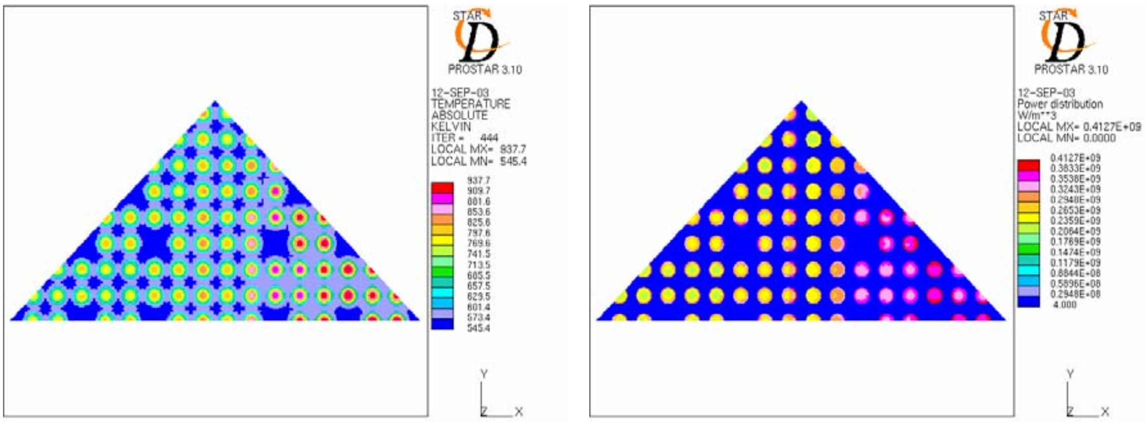


Fig.5 Coupling Mechanics: Interface Design

6. Coupled Calculations

Demonstration of the integrated analysis capability has been initiated for a series of sample problems. The initial test problem was a simple 3 by 3 pin system, containing UO2 and MOX pins and a central guide tube. Results illustrated expected temperature differences between the fuel types and asymmetric heating and cooling, as well as the effects on the power distribution of self-shielding. Test results have also been performed for a "mini-core" problem, representing 4 quadrants of adjacent assemblies of different types. Results such as those indicated in Figure 6 show the calculation of the expected asymmetry in the power and temperature distributions. Detailed examination illustrated the important effect of properly treating the temperature distribution within the fuel pin. Computational results on the JAZZ multiprocessor Linux cluster at Argonne indicate that extrapolation of such calculation to whole core application can be accomplished with current generation high performance computer systems. Preliminary estimates indicated that steady state calculation of prototypic PWR cores can be performed on a teraflop class machine in less than a day. Extrapolation of these estimates suggest that transient calculations for relevant scenarios can be also be accomplished in computing times of several tens of hours on such machines. Scalability of results to date also indicates that expected availability of more powerful machines will result in proportional reduction in computing time, with the expectation that such whole core high fidelity calculations will soon be possible in times measured in hours, rather than days or week.



Temperature Distribution Power Distribution

Fig.6 Mini-Core Model: Results

7. Conclusion

Current activities in this project are focused on implementation of transient neutronics capabilities, continued validation of CFD models, integration of CFD with thermo-mechanics and performance of integrated calculations. The integrated calculations will focus on improvement to the numerical iteration strategy for the multi-physics problem, to reduce the overall computing time for steady state and transient problems. In addition, validation of the integrated capability against standard benchmark problems is being assessed. Such analyses will not only confirm the ability of this analysis system to calculate correctly the integral measures being compared, but also demonstrate the ability to predict important detailed information at the sub-pin and sub channel level that may be important in assessing safety characteristics or increasing performance, without reduction in true safety margins.

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